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Kinetic temperature relaxation and nonequilibrium fluctuations in two-dimensional Lennard–Jones systems during nonstationary heat transfer

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Abstract. The kinetic temperature fluctuations in two-dimensional Lennard–Jones systems are compared under equilibrium and nonequilibrium conditions. The calculated relaxation times of the kinetic temperature to the steady state are of the order of 10^{-11} s and their values decrease with the energy increasing. It is shown that the distribution functions of the relative fluctuations have the form of Gaussian type, the dispersion in a nonsteady state is more than in a steady one. The characteristic times of the fluctuations decay to the steady state levels are in agreement with the typical characteristic times of nonlocal molecular dynamics models describing nonstationary heat transfer.

1 Introduction

One of the problems of nonequilibrium thermodynamics is the description of the conductive nonstationary heat transfer. To solve the infinite velocity paradox the phenomenological Cattaneo model [1] was proposed in the middle of the 20th century. In this nonlocal model is entered the relaxation time τ_v into the Fourier's law

$$\boldsymbol{q}(\boldsymbol{x},t)+\tau_v\frac{\partial q(\boldsymbol{x},t)}{\partial t}=-\lambda(T)\nabla T(\boldsymbol{x},t), \tag{1}$$

where $T(\boldsymbol{x},t)$ is the temperature, $\boldsymbol{q}(\boldsymbol{x},t)$ the heat flux, and $\lambda(T)$ is the thermal conductivity. As a consequence, the classical heat transfer equation of parabolic type is transferred into the hyperbolic type telegrapher equation with a finite velocity of the thermal perturbations propagation.

The same procedure can be applied to the Fick's law for diffusion. As a result, one can proceed to various nonlocal models, in particular, within the framework of extended thermodynamics [2–7] and to complex Brownian movement models [8]. It should be noted that the non-local equations in the form (1) are also approximations. The author of the paper, for instance, proposed to use the new approximation with the correction function $F(x,t)$ [9] for the purpose of a more correct estimation of the relationship between the flux (J) and the concentration gradient in a one-dimensional case for the Fick's law

$$J+\tau\partial J/\partial t=-DF(x,t)\nabla C(x,t). \tag{2}$$

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Here J is the particles flux, C the concentration, D the diffusion coefficient, and τ is the relaxation time in random walk model [9], analogous to τ_v in (1). However, the introduction of the relaxation times and their calculation require justification. It can be done based on first principles using the molecular dynamics (MD) simulation. It is convenient to use the Lennard–Jones interacting particles in this case. Such estimates and calculations were made for the modified Fourier's law models [10–14] in three-dimensional and two-dimensional systems [15,16]. It was shown that the characteristic times τ_v in (1) lie in the range of 10^{-11}–10^{-12} s [17,18] for solid argon. In this paper, we attempt to estimate similar times based on the relaxation and fluctuation properties of the Lennard–Jones systems.

It should be emphasized that the processes under consideration are a demonstration of the random forces action [19,20] and are founded on a deep interrelation of the fluctuations and dissipative processes [21]. These processes can also be viewed from the standpoint of dynamical chaos [22], solving the irreversibility problem [23], ergodicity [24], heat fluxes in Hamiltonian systems [25], thermal relaxation [26], deviations from the linear response theory [27], the fluctuation-dissipation theorem [28,29], and the temporal asymmetry of fluctuations in nonequilibrium systems [30], in low-dimensional systems [31,32]. The several different temperatures arising in non-equilibrium steady states were discussed in [33–36], the cases with high fluctuation energy in non-equilibrium steady state were discussed in [37–39], and other interesting aspects of nonlocal heat transfer were discussed in [40–43].